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Computational modeling of the transverse-isotropic elastic properties of single-walled carbon nanotubes

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ABSTRACT

Various experimental and theoretical investigations have been carried out to determine the elastic properties of nanotubes in the axial direction. Their behavior in transverse directions, however, has not been well studied. In this paper, a combination of molecular dynamics (MD) and continuum-based elasticity model is used to predict the transverse-isotropic elastic properties of single-walled carbon nanotubes (SWCNTs). From this modeling study, five independent elastic constants of an SWCNT in transverse directions are obtained by analyzing its deformations under four different loading conditions, namely, axial tension, torsion, uniform and non-uniform radial pressure. To find the elastic constants in the transverse directions, the strain energy due to radial pressure is calculated from the MD simulation. Then, a continuum-based model is implemented to find the relation between the strain energy and maximum pressure under these two loading conditions. Based on the energy equivalence between the MD simulation and the continuum-based model, the transverse-isotropic elastic constants of SWCNTs are computed. The effectiveness of this approach is demonstrated by comparing the results with previous experimental and computational works.

1. Introduction

Carbon nanotubes (CNTs) are quasi-one-dimensional nanostructures that have attracted considerable attention in the fields of mechanics, electronics, physics and chemistry. It has been theoretically and experimentally confirmed that CNTs possess exceptionally high stiffness and strength. Their stiffness and strength are in the order of 1 TPa and 200 GPa, respectively [1]. Studying the mechanical behavior of CNTs is important considering the broad field of applications predicated for them such as in nano-sized strain sensors and actuators, nanofluidic components, and as reinforcement agents in nanocomposites. Various experimental and theoretical studies have been performed to determine the mechanical properties of single-walled carbon nanotubes. It is to be noted that many simulation techniques such as molecular dynamics (MD) and molecular mechanics methods, based on prescribed empirical potentials [2–4], tight-binding-based approaches [5], first principles quantum mechanical methods [6], and structural mechanics models [7,8] have been used to predict the isotropic elastic properties, such as Young's modulus, major Poisson's ratio and shear modulus of SWCNTs [9].

The in-plane stiffness of graphite has been determined experimentally to be 1.06 TPa, whereas its stiffness in the direction perpendicular to the layers is only 0.036 TPa [10]. Similarly, the transverse Young's modulus of a CNT is expected to be much smaller than its axial one. While the multi-walled carbon nanotubes have an axial Young's modulus of ~2 TPa [11], they show reduced stiffness in their transverse directions [12]. SWCNTs are even softer than multi-walled nanotubes in transverse directions [13]. TEM observations show that when two nanotubes are brought close to each other, the contact area is flattened due to van der Waals forces between them [14]. Lordi and Yao [15] utilized HRTEM in tandem with MD simulations to study the mechanical force–displacement relationship of SWCNTs. Their results revealed that large radial compressions could be induced by a small force on nanotubes.

Relatively few studies have been devoted to analyze the elastic behavior of these nanostructures in transverse directions. Lu [10] used an empirical force-constant model and Lennard–Jones potential to investigate the effect of radius, helicity and number of walls on the transverse-elastic properties of carbon nanotubes and nanoropes. It has been proposed that CNTs can be modeled as

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transverse-isotropic materials [16–20]. Shen and Li [19,20] found closed-form solutions for five independent elastic constants of a carbon nanotube as a transverse-isotropic material. In their work, an energy approach based on molecular mechanics was used to evaluate the local and global deformations of SWCNTs and MWCNTs. This was carried out under four loading conditions, namely axial tension, torsion, in-plane biaxial tension, and in-plane pure shear, and yielded closed-form expressions for the longitudinal Young's modulus, major Poisson's ratio, longitudinal shear modulus, plane strain bulk modulus, and in-plane shear modulus. In addition, Jin and Yuan [21] used MD simulations to study the transverse-elastic properties of SWCNTs. Using energy and force approaches, they calculated the transverse elastic constants of SWCNTs. Moreover, Wang et al. [22] determined the five elastic constants via a thin-shell model together with MD simulations and showed that these transverse-elastic properties significantly depend on the size and chirality of the CNT.

To properly use CNTs in nanoelectromechanical and nanoelectronic systems, knowledge of their transverse deformability is as important as that of their longitudinal properties [23]. It has been shown that the radial deformation of CNTs may strongly affect their electrical properties [24,25]. Also, the elastic properties of a CNT in the transverse directions significantly affect the mechanical integrity of nanowire templates, hydrogen containers, nanogears, and nanofluidic devices using CNTs as structural components [26]. Furthermore, the transverse elasticity of CNTs plays an important role in the interfacial stresses and failure behavior of CNT-reinforced nanocomposites. It is to be noted that because of their high strength and stiffness, as well as high aspect ratio and low density, carbon nanotubes are considered as ideal reinforcement elements in the new generation composites. The proper use of CNTs as reinforcement agents in composites with anisotropic properties and subject to loading conditions in different directions requires data on mechanical properties of CNTs in all directions, especially the transverse ones, and not just in the axial directions. Our motivation has been to derive the mechanical properties of nanotubes in transverse directions so that when these tubes are used as reinforcement elements in nanocomposites under various types of applied loads, the appropriate directional properties of CNTs can be included in the computations.

The objective of this paper is to formulate a transverse-isotropic elastic model of SWCNTs that combines methods from continuum elasticity theory and molecular dynamics simulation. This model is employed to predict the transverse-elastic properties of SWCNTs. To achieve this end, MD simulations are used to model the mechanical behavior of SWCNTs under axial, torsional and radial loadings. Also, continuum-based models using the linear elasticity theory are employed to model the mechanical behavior of SWCNTs under these loading conditions. The methodology developed herein combines a unit cell continuum model with MD simulations to determine the transverse-isotropic elastic constants of SWCNTs. The predicted elastic constants are compared with the available published data.

2. Modeling

2.1. Analysis methodology

As discussed before, SWCNTs exhibit transverse-isotropic properties in the plane normal to their longitudinal axis. Transverse-isotropic materials possess a unique axis about which the material's elastic properties are independent of direction [27]. With this type of material symmetry, the number of independent elastic constants in the elasticity tensor is reduced to 5 from a total of 21 independent constants in the case of a fully anisotropic solid. Adopting the coordinate system shown in Fig. 1 for an SWCNT, the strain–stress relations can be written in the matrix from:

$$\begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{yz} \\ \varepsilon_{zx} \\ \varepsilon_{xy} \end{Bmatrix} = \begin{bmatrix} S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{13} & 0 & 0 & 0 \\ S_{13} & S_{13} & S_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44}/2 & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44}/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{11}-S_{12} \end{bmatrix} \begin{Bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{zx} \\ \sigma_{xy} \end{Bmatrix} \quad (1)$$

Regarding the Poisson's ratio, Young's modulus and shear modulus in the longitudinal direction and the Poisson's ratio and Young's modulus in the transverse plane; namely v, E, G, v', and E', respectively, the following relations for the engineering elastic constants of a transverse-isotropic solid are obtained:

$$S_{11} = \frac{1}{E'} \quad S_{12} = -\frac{v'}{E'} \quad S_{13} = -\frac{v}{E} \quad S_{33} = \frac{1}{E} \quad S_{44} = \frac{1}{G} \quad (2)$$

These are the five elastic constants to be determined. To compute these constants, MD simulations were performed under four different loading conditions, namely; axial tension, torsion, uniform and non-uniform radial pressure as schematically shown in Fig. 2. As was previously mentioned, Shen and Li [19,20] developed an energy approach in the framework of molecular mechanics to derive a set of closed-form expressions for local and global deformations of CNTs. To obtain the transverse properties, they used in-plane biaxial tension and in-plane pure shear tests.

Here, a new method is proposed based on the combination of MD simulation and continuum-based elasticity theory to determine the SWCNT transverse elastic constants. The model is based on the Cauchy–Born rule, which relates the deformation behavior of a continuum to the deformation behavior of the crystal lattice of a material [9]. Each point in the continuum is enveloped within a representative cell in which the deformation is uniform, and the strain-energy density in the continuum level is computed by summing the energies of all the interatomic bonds contained within that cell, after the deformation is applied. The methodology involves applying a uniform and non-uniform radial pressure to an SWCNT and then computing the potential energy due to interatomic interactions as a function of the imposed pressure. A direct transformation to continuum properties is then made by assuming that the potential energy density of discrete atomic interactions is equal to the strain-energy density of the continuous substance occupying the volume of the SWCNT. In this way, the relations between the imposed pressure and the strain energy of the equivalent solid are obtained. These relations yield the Poisson's ratio

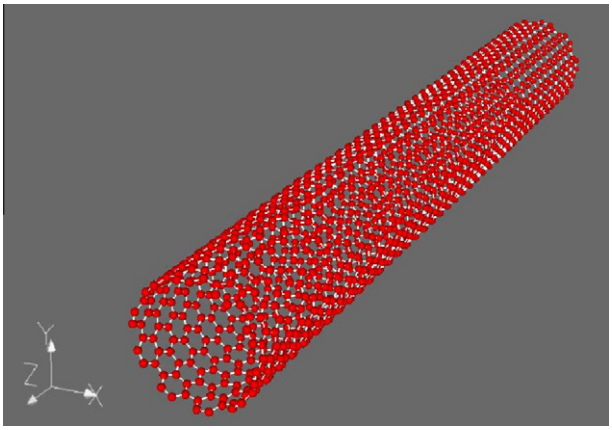

Fig. 1. Nanotube coordinate system.